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Hydrogenic Impurities in Quantum Dots and Wires

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(APPLIED MATHEMATICS)

By

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Abstract

The binding energy of a hydrogenic impurity in a single Spherical Quantum Dot (SQD) has been calculated by utilizing techniques that differ from those used in our earlier work. In off-central and central impurities the time independent perturbation theory has been applied in the case of parabolic confining potential. The inverse distance between the electron and the center of the impurity has been expanded as a series in Legendre Polynomials and spherical harmonics. Also, the Asymptotic Iteration Method (AIM) has been investigated with a confining potential that consists of three terms. The first term stands for the potential due to central impurity while the last term represents the parabolic potential. The (AIM) has been applied to determine the binding energy of a central impurity. This has not been done hitherto. The ground state and the first approximation agree entirely with the result of the perturbation technique while the second approximations of both methods differ by about 16.5 % which is quite reasonable.

The exact solutions of the radial Schrödinger equation have been investigated subject to specific confining potentials. The results of all earlier treatments have been modified and extended to include the second node solutions.

The case of multilayered spherical quantum dot (MSQD) in the presence of a central impurity has been explored. The confining potentials have been taken to be finite or parabolic. In the latter case an analytical approach has been utilized to obtain the solution unlike an earlier treatment (Akgül *et al* [4]) where an entire numerical technique has been applied. In the presence of the central impurity, the asymptotic iteration method (AIM) has been employed to obtain the solutions in the dot regions. This is one of the main aims of the thesis. In fact, the AIM has not been used before to deal with such type of problems. The results obtained for the hydrogenic binding energy in the ground state 0S (l=0) consistent to a great extent with the corresponding results of Akgül *et al* [4]. The calculations have confirmed strongly the importance of the AIM in solving problems of complicated potential energies.

Keywords:

Quantum Dots and Wires, Central and Off Central Hydrogenic Impurities, Parabolic and Finite Confining Potentials, Ground and Excited Energy States, Impurity Binding Energy, Perturbation Techniques, Asymptotic Iteration Method, Exact Solutions of the Radial Schrodinger Equations, Multilayered Spherical Quantum Dots.

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Introduction

1.1 Review of Hydrogenic Impurities in Quantum Dots and Wires

Low dimensional semiconductors have great importance in practical life as they enter in many modern electronic industries such as radio, computer, telephone, television, transistor solar cells and solar panels are examples of semiconductor devices where light energy is converted to electrical energy.

In the last three decades the physics of low dimensional semiconductors have been speculated by many scientists along different directions. A low dimensional system is a system where the motion of charge carriers (mainly electrons) is restricted in one or more directions by some confining potentials. The confinement of charge carriers in low dimensional structures affects substantially their density of states and the strength of Coulomb interactions with impurities. Accordingly the binding energy of a hydrogenic impurity has gained a great attention and has become an important field of study in low dimensional nanostructures.

The field of low dimensional structures started in two dimensional (2D) superlattices and quantum wells. More recently, other lower dimensional structures such as one dimensional (1D) quantum wires and zero dimensional (0D) quantum dots have attracted a great attention. The studies have also been extended to consider more complicated nanostructures such as coaxial quantum wires and multilayered spherical quantum dots.

The calculation of the binding energy of a hydrogenic impurity in a quantum well (QW) has started by the work of Bastard [10]. He considered the simple case

of an infinite confining potential quantum well in the case of central and off-central impurity. He applied the variational method with a trial wave function that depended on one variational parameter. The case of finite confining potential quantum well was, then, studied by Chaudhuri and Bajaj [23] by extending the approach used in Bastard [10]. The finite confining potential has led to the appearance of the tunneling effect which causes the binding energy to be maximum for a quantum well of a certain width. Furthermore, Chaudhuri and Bajaj [23] investigated the effect of nonparabolicity on the energy levels of the impurity.

In the case of central impurity Zhu [103], Greene and Bajaj [35] and Mailhiot *et al* [61] introduced more complicated variational methods. In Ref. [61] the authors dealt with the case of finite confining potential quantum well by expanding the trial wave function in terms of Gaussian type orbital functions in the presence and absence of the impurity. They further, took, into consideration the different masses and dielectric constants of the well and barrier. Their treatment was extended in a more accurate manner by Fraizzoli *et al* [33] where a different basis for the expansion of the trial wave function was utilized. Elabsy [31], Akbas *et al* [2, 3] and Hakimyfard [36] studied the effect of the temperature and hydrostatic pressure on the effective mass, confining potentials, dielectric constants and consequently on the calculated binding energies.

Tanaka *et al* [87, 88], Oliveira [78] and Mikhail and Ismail [66] considered the case of an off-central impurity in a finite confining potential well. In [87], [78] the calculations were carried out numerically. However, in Mikhail and Ismail [66], analytical expressions for the energy variational eigenvalues and binding energy were obtained. The analytical expressions were then utilized to infer useful

information regarding the initial deviation from the result of infinite confining potential well and to derive some other important parameters.

In most of the above references the binding energy of the impurity in the ground state was only considered. The binding energy of four excited states of a central impurity has been calculated for a finite confining potential well by Greene and Bajaj [35], Chaudhuri and Bajaj [23]. Also, the effect of magnetic and electric fields on the ground state binding energy in quantum wells have been investigated by Kasapoglu *et al* [50, 51] , Kasapoglu [52] and Barseghyan *et al* [9].

For a single quantum well wire (QWW), Lee and Spector [55] calculated the binding energy of an axial hydrogenic impurity in an infinite circular wire with an infinite confining potential. Brown and Spector [16] extended their results to consider the case of finite confining potentials and an off-axial impurity. The effect of donor and acceptor impurities on the optical properties of quantum well wires was also investigated by Montenegro *et al* [74], [75] and Santhi and Peter [84]. Moreover, Branis *et al* [15], have studied the binding energy of an axial hydrogenic impurity in QWWs with infinite and finite confining potentials in the presence of an axial magnetic field. Similar studies were also performed in Merchancano and Marques [63], Niculescu *et al* [77], Manaselyan *et al* [62], Karki *et al* [47] and Mikhail and El Sayed [68]. In the last reference the variational method was applied with a new form of the trial wave function which has the advantage of satisfying the required boundary conditions in the case of different effective masses of wire and barrier.

The excited states, binding and transition energies of impurities in QWWs have been considered within the framework of the variational method by Latge *et al* [54] and Villamil *et al* [91], [92]. In these studies the effective masses of the

well wire and barrier are assumed to be equal and no analytical expressions for the binding energy of the ground and exited states have been derived. Mikhail and El Sayed [68] have derived new analytical expressions for the binding energy of the ground and first four excited states in the presence of an axial magnetic field for different effective masses of the wire and barrier. Also, the effect of an external electric field on the binding energy of axial and off-axial impurities in QWWs was explored in Mikhail and Emam [65] and Wang *et al* [94].

The study of quantum systems with time depended masses and time dependent magnetic and electric fields presents a very important problem in quantum physics. The invariant operator method is a very powerful technique to solve such problem. This method has been initially introduced by Lewis [56], [57] and Lewis and Riesenfeld [58]. Choi [22] utilized this method with some other unitary transformations to investigate the exact quantum states of a one dimensional quantum well wire. He succeeded in inverting the time dependent Schrödinger equation to the equation of a one dimensional harmonic oscillator of constant mass. Moreover, Sharma [86] has explained the time dependent impurity in a quantum well wire. He has considered the spin transport and probing stable phases of single impurity where the parametric pumping is developed by studying the quantum wire with a time dependent impurity potential.

The binding energy of hydrogenic impurities in the more complicated coaxial quantum well wires (CQWW) has, also, been considered. Zeng *et al* [100], Mikhailov *et al* [73], Aktas *et al* [5], [6] and Boz and Aktas [13] have investigated such problem in the presence of external electric and magnetic fields. Boz and Aktas [13] and Aktas *et al* [6] explored a CQWW of two $GaAs$ wires and two

$Ga_{1-x}Al_xAs$ barriers. They have calculated the binding energy of axial and off-axial impurities in the presence of an axial uniform magnetic field or in the presence of an electric field perpendicular to the axis of symmetry. They applied the fourth order Runge-Kutta numerical method to solve the Schrödinger equation in the absence of impurity. The variational technique has then been utilized to calculate the impurity energy ground state and the corresponding binding energy. Mikhail and El Sayed [69] considered the same geometry of CQWW used in the previous two references. They have taken into account the different effective masses in the different regions of the CQWW. Also, in the absence of impurity the exact analytical solutions of the radial Schrödinger equation in the different regions have been derived in terms of the hypergeometric and confluent hypergeometric functions. The involved coefficients as well as the energy eigenvalue have been obtained by solving the boundary conditions at the interfaces between the different regions. In the presence of the impurity, the variational method has been applied by using a new trial wave function which has the advantage that it satisfies the required boundary conditions in the case of different masses. It thus resembles the exact solution in this respect and has led to a considerable improvement of the results.

For a single quantum dot (QD), the binding energy of a central impurity has been investigated by using three different approaches. In the first approach Zhu [103] and Zhu *et al* [104] have obtained the exact wave functions and energy eigenvalues by using a series solution. In some cases, however, the convergence of the series becomes slow. As a remedy for this difficulty Zhu *et al* [103,106] used uniformly convergent Taylor expansions around a number of radial distances outside the dot. Alternative techniques to derive the exact solution of the

Schrödinger equation in the presence of a central impurity have been considered by Chuu *et al* [24], Yang *et al* [98] and Goldman and Joslin [34]. Also, Holovatsky *et al* [40, 41] have expressed the solution in terms of the Whittaker functions which can then be expressed in terms of the confluent hypergeometric functions. In most of the above references a distinction has been made between the form of the wave function in the two cases of –ve and +ve electron energy. On the other hand, the electron energy is always determined from the boundary conditions which depend on the form of the wave function. This, in turn, gives rise to a difficulty in choosing the required case.

The second approach is based on the variational method. This approach has the advantage that it can also be applied in the case of off-central impurity. Montenegro and Merchancano [76] applied this method with the conventional form of the trial wave function that consists of a part that represents the exact solution in the absence of impurity and a part that represents the impurity with a variational parameter involved. The same approach was also used by Peter [81], Dane *et al* [28, 29] and by Akbas *et al* [2]. In Ref. [81] the effect of the hydrostatic pressure has been included while in Refs. [2, 29, 81] the effect of the electric and magnetic fields were taken into consideration. A modified variational optimization approach for the central impurity in a QD has been introduced by Cakir *et al* [19], [20], Őzmen *et al* [79] and by Yakar *et al* [96, 97]. In this method the wave functions were expanded in terms of Slatar – type orbital functions with the coefficients as variational parameters.

The third approach is the strong perturbation technique that was introduced originally by Jiang [45] and was applied for the calculation of the binding energy of a central impurity in a QD by Kassim [53]. However, Mikhail and Ismail [71]

discussed the second and third approaches and showed that the variational method leads to better results than the strong perturbation technique and is accordingly more powerful.

Regarding, off-central impurities in quantum dots, the corresponding Schrödinger equation cannot be solved exactly. In view of this the variational method has been applied with different forms of the trial wave function. Zhu and Chen [105] used a trial wave function in the form of linear expansion where the coefficients have been taken as the variational parameters. For an off central impurity inside the dot, the basis of expansion was taken to be the series solution exact eigenfunctions obtained in the case of central impurity. A different basis was utilized for an impurity located outside the dot. Alternative, forms for the trial wavefunctions were employed in Wang and Yang [93], Merchancano *et al* [64] and Mikhail and Ismail [67]. In the last reference the trial wave function was taken in the same type as that used in Montenegro and Merchancano [76]. Mikhail and Ismail [67] have derived analytical expressions for the energy expectation value and for the binding energy of an off-central impurity. Moreover, they have further explored the importance of their analytical expressions in determining some valuable parameters. Some approaches other than the variational method have also been utilized to calculate the binding energy of an off central impurity in a spherical QD. Lima *et al* [59] used a model in which the Coulomb interaction between the electron and hydrogenic impurity is replaced by a projection operator. Also, villalba *et al* [89, 90] applied an alternative numerical method.

Some other related works have been considered in Partima and Shivani [80] where the optical properties of an undoped and magnetic impurity doped